Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 12:42 AM EDT

PDB ID	:	6OBH
Title	:	Structure of HIV-1 CA 1/2-hexamer
Authors	:	Summers, B.J.; Xiong, Y.
Deposited on	:	2019-03-20
Resolution	:	2.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10070 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1692	1064	296	319	13			
1	D	214	Total	C	N	O	S	0	0	0
			1665	1048	291	314	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP T2CI25
A	14	CYS	ALA	engineered mutation	UNP T2CI25
A	184	ALA	TRP	engineered mutation	UNP T2CI25
A	185	ALA	MET	engineered mutation	UNP T2CI25
D	0	MET	-	initiating methionine	UNP T2CI25
D	14	CYS	ALA	engineered mutation	UNP T2CI25
D	184	ALA	TRP	engineered mutation	UNP T2CI25
D	185	ALA	MET	engineered mutation	UNP T2CI25

- Molecule 2 is a protein called CA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1660	1045	291	311	13			
2	E	220	Total	C	N	O	S	0	0	0
			1687	1061	296	316	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP B6DRA0
B	45	CYS	GLU	engineered mutation	UNP B6DRA0
B	54	CYS	THR	engineered mutation	UNP B6DRA0
B	184	ALA	TRP	engineered mutation	UNP B6DRA0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	185	ALA	MET	engineered mutation	UNP B6DRA0
E	0	MET	-	initiating methionine	UNP B6DRA0
E	45	CYS	GLU	engineered mutation	UNP B6DRA0
E	54	CYS	THR	engineered mutation	UNP B6DRA0
E	184	ALA	TRP	engineered mutation	UNP B6DRA0
E	185	ALA	MET	engineered mutation	UNP B6DRA0

- Molecule 3 is a protein called CA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total	C	N	O	S	0	0	0
			1692	1064	296	319	13			
3	F	214	Total	C	N	O	S	0	0	0
			1665	1048	291	314	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP T2CI25
C	42	CYS	ALA	engineered mutation	UNP T2CI25
C	184	ALA	TRP	engineered mutation	UNP T2CI25
C	185	ALA	MET	engineered mutation	UNP T2CI25
F	0	MET	-	initiating methionine	UNP T2CI25
F	42	CYS	ALA	engineered mutation	UNP T2CI25
F	184	ALA	TRP	engineered mutation	UNP T2CI25
F	185	ALA	MET	engineered mutation	UNP T2CI25

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	2	Total	Na	0	0
			2	2		
4	D	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0
5	E	1	Total O 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.77Å 77.75Å 77.76Å 70.65° 70.70° 70.59°	Depositor
Resolution (Å)	45.00 – 2.96	Depositor
% Data completeness (in resolution range)	92.5 (45.00-2.96)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.12_2829	Depositor
R, R_{free}	0.208 , 0.265	Depositor
Wilson B-factor (Å^2)	94.5	Xtriage
Anisotropy	0.173	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.448 for k,l,h 0.448 for l,h,k 0.040 for -h,-l,-k 0.040 for -k,-h,-l 0.041 for -l,-k,-h	Xtriage
Total number of atoms	10070	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.